

ABSTRACT OF THE DISCLOSURE

A method for identifying a ligand of a target macromolecule is disclosed, comprising the steps of: soaking one or more crystals of the target macromolecule in a solution containing a collection of compounds generated in situ or separate from the crystal, where the solution has been prepared without the purification of the synthesized collection of compounds; obtaining an X-ray crystal diffraction pattern of the soaked macromolecule crystal; and using said X-ray crystal diffraction pattern to identify any compound bound to the macromolecule crystal, said compound being a ligand of the target macromolecule.